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Order Parameter Symmetry in Doped YBCO Systems

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Abstract

Intense experimental and theoretical efforts have recently been brought to bear on the determination of the symmetry of superconducting order parameter in high T_c Cuprates as this would shed light on the nature of microscopic interactions that are responsible for superconductivity in these unusual systems. We use a two band model that reproduces the Fermi surface seen in ARPES experiments of Shen et al.,[1] and study the symmetry of order parameter in the YBCO system. The model incorporates the effects of tunnelling in the c-direction between the planes and chains of these Cuprates. It is observed that a suitable choice of the phase of the pair wave-function in the planes and chains lead to both s- and d-wave like features. We calculate the detailed phase diagram of this system, observe the shift in the position of the node(s) of the order parameter(s) on the Fermi surface with doping and explain the seemingly contradictory experimental observations about the presence of both s- and/or d-wave symmetry[2] in these systems.

Quite a large number of experiments backed by careful calculations have been brought to bear upon the resolution of the seemingly irreconcilable and contradictory observations about the nature of symmetry of the superconducting order parameter (OP) in the Cuprate superconductors[2]. An understanding of this symmetry, which is still unresolved, will shed considerable light on the nature of the pairing mechanism(s) in these unusual systems.

Broadly, there are several classes of experiments that probe the symmetry of OP in the cuprates: i) Transport and thermodynamic measurements[3], notably the temeperature dependence of the London penetration depth (λ)[4] that show a linear temperature dependence

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of λ, indicating that at low energies the density of superconducting states (SDOS) varies linearly with energy in pure samples, a signature of gapless excitations. ii) Angle resolved photoemission experiments[5] that show a node (with a small offset) along the (π, π) direction of the square Fermi surface (FS)of $YBa_2Cu_3O_7$. iii) Josephson measurements: magnetic field dependence of dc SQUID[6, 7] predict a π phase shift consistent with d-wave scenario. Conversely, c-axis Josephson tunneling[8] between twinned and untwinned $YBa_2Cu_3O_7$ and Pb junction finds a Josephson current, albeit small, indicative of a symmetric OP. Recent atomic forced microscopy measurements of Kitazawa and his group[9] found evidence of gap everywhere on the FS in Bi-2212 materials. Critical current between a hexagonal grain and its surroundings is found to be non-zero[10] and it scales with the number of sides engaged, consistent with the presence of a conventional s-wave component. iv) Sensitivity of superconducting T_c with elastic scattering is found to be too weak (follows, instead, the Ioffe-Regel criterion, $k_f l = 1$, where l is the mean-free path of the electrons) to conform to the behaviour of a pure d-wave symmetry[11].

While there is a general concensus that there are nodes on the FS in all the hole-doped Cuprates, there is, however, no consensus about its origin. Models based on spin fluctuation[12] predict a $d_{x^2-y^2}$ symmetry for the OP, while an interlayer tunneling-enhanced conventional superconductivity scenario[13] envisages extremely anisotropic s-wave gap function. It is also useful to note that the symmetry of YBCO system is orthorhombic and not tetragonal, so an admixture of s- and d-components is inescapable[14], and the nomenclature is based on the dominance of one component over the other.

In view of this conflicting scenario it is useful to look for models that incorporate i) the essence of the band structure of the system concerned and ii) reproduce much of the experimentally observed features. Comberscot and Leyronas[15] have tried to incorporate the fact that in YBCO systems, the existence of both chains and planes can have a strong bearing on the nature of pairing wave function that occurs. We use a similar model and show that it is indeed possible to reproduce many of the experimentally observed features of the OP without explicitly considering a d-wave pairing function and features consistent with both d- and s-wave are obtainable with a suitable choice of the relative phase of two isotropic pairing functions residing mainly on the plane and chain derived bands.

We consider the Hamiltonian: $H = H_0 + H_I$ where,

$$H_0 = \sum_{\mathbf{k}\sigma} [\epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \epsilon'_{k_y} d^\dagger_{k_y\sigma} d_{k_y\sigma} + t(d^\dagger_{k_y\sigma} c_{\mathbf{k}\sigma} + h.c.)] \tag{1}$$

$\epsilon_{\mathbf{k}}$ and ϵ'_{k_y} are energy dispersions, and $c_{\mathbf{k}\sigma}, d_{\mathbf{k}\sigma}$ are destruction operators for electrons in the plane and the chain respectively. The off-diagonal term t is small ($t \approx 50\ meV$)[16], momentum independent and introduces band interaction. This implies that in $YBCO$ system, an electron is never in a true eigenstate of planes or chains, rather, it has components on both the bands. This term shows up in the band-crossing region leading to anticrossing features with two sheets of the FS as seen in $YBCO$. Thus moving along a given sheet of the FS, an electron changes its character from being in the plane band to being in the chain band. This feature has its bearing on the relative sign of the OP as we discuss below.

In order to fit our band structure with a realistic one obtained from the ARPES data[5] for the $YBCO$ system, we take five nearest neighbour hopping parameters in the plane, in both a and b direction and two nearest neighbours in the chain. The dispersion relation in the plane is now

$$\begin{aligned}\epsilon_{\mathbf{k}} &= -\mu_p - 2t_1 Cos(k_x) + Cos(k_y) + 4t_2 Cos(k_x)Cos(k_y) \\ &- 2t_3 Cos(2k_x) + Cos(2k_y) - 4t_4[\ Cos(2k_x)Cos(k_y) \\ &+ Cos(k_x)Cos(2k_y)\ ] + 4t_5 Cos(2k_x)Cos(2k_y) \end{aligned} \tag{2}$$

and in the chain

$$\epsilon'_{k_y} = -\mu_c - 2h_1 Cos(k_y) + 2h_2 Cos(2k_y) \tag{3}$$

The resulting FS, shown in Fig. 1, very closely resembles the observed FS[5] and the position of the van Hove singularities (about $10meV$ away from the FS[17]) seen in $YBa_2Cu_3O_7$, with the following choice of the hopping parameters ,
$[\mu_p, t_1, ..., t_5] = [-290, 300, 100, 25, 25, 20]meV$ and $[\mu_c, h_1, h_2] = [-740, 530, 135]meV$.

The non-interacting Hamiltonian H_0 can be easily diagonalised by the introduction of new quasiparticle operators $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ defined by

$$\begin{pmatrix} c_{\mathbf{k}\sigma} \\ d_{\mathbf{k}\sigma} \end{pmatrix} = \begin{pmatrix} \frac{t}{\sqrt{t^2+(\epsilon^+-\epsilon)^2}} & \frac{\epsilon^- - \epsilon'}{\sqrt{t^2+(\epsilon^- - \epsilon')^2}} \\ \frac{\epsilon^+ - \epsilon}{\sqrt{t^2+(\epsilon^+-\epsilon)^2}} & \frac{t}{\sqrt{t^2+(\epsilon^- - \epsilon')^2}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}\sigma} \\ \beta_{\mathbf{k}\sigma} \end{pmatrix}, \tag{4}$$

The quasiparticles corresponding to $\alpha^\dagger_{\mathbf{k}\sigma}(\beta^\dagger_{\mathbf{k}\sigma})$ live on the upper (lower) FS given by $\epsilon^+ = 0(\epsilon^- = 0)$, where $\epsilon^\pm = \frac{1}{2}(\epsilon + \epsilon') \pm \sqrt{(\epsilon - \epsilon')^2 + 4t^2}$ denote the dispersions of the two quasiparticle bands and the $\mathbf{k}$-dependences have been omitted for notational convenience. Fig. 1 shows the corresponding FS in the first quadrant of the Brillouin zone (BZ) and Fig. 2,

the partial and total density of states (DOS) with the van Hove singularities predominantly located about $10meV$ below the FS[17].

Superconductivity occurs through the interaction part of the Hamiltonian[18]

$$\begin{aligned} H_I &= -g\sum_{\mathbf{kk'}} c^\dagger_{\mathbf{k'}\uparrow}c^\dagger_{-\mathbf{k'}\downarrow}c_{-\mathbf{k'}\downarrow}c_{\mathbf{k}\uparrow} - g'\sum_{\mathbf{kk'}} d^\dagger_{\mathbf{k'}\uparrow}d^\dagger_{-\mathbf{k'}\downarrow}d_{-\mathbf{k'}\downarrow}d_{\mathbf{k}\uparrow} \\ &\quad +K\sum_{\mathbf{kk'}}\left(d^\dagger_{kp\uparrow}d^\dagger_{-\mathbf{k'}\downarrow}c_{-\mathbf{k'}\downarrow}c_{\mathbf{k}\uparrow} + h.c.\right) \end{aligned} \tag{5}$$

where g and g' are the pairing interactions (attractive, non-retarded) in the plane and chain respectively; K is the measure of pairing interaction between plane and chain and is assumed repulsive. It is this repulsive interaction that forces the quasiparticles in planes and chains to stay away in real space forcing $\sum_{\mathbf{k}}\langle c_{\mathbf{k}\sigma}d_{-\mathbf{k}-\sigma}\rangle \simeq 0$ which requires the pairing wave function to have nearly equal regions of positive and negative signs in the BZ.

A simple BCS mean-field theory gives the following Hamiltonian,

$$H^{mf}_I = \sum_{\mathbf{k}}\left[\Delta c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} + \Delta' d^\dagger_{\mathbf{k}\uparrow}d^\dagger_{-\mathbf{k}\downarrow} + h.c.\right] + \Delta^*\frac{K\Delta' + g'\Delta}{gg' - K^2} + \Delta'^*\frac{K\Delta + g\Delta'}{gg' - K^2} \tag{6}$$

where Δ, Δ' are defined by,

$$\Delta = -g\sum_{\mathbf{k}}\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle + K\sum_{\mathbf{k}}\langle d_{-\mathbf{k}\downarrow}d_{\mathbf{k}\uparrow}\rangle$$

$$\Delta' = K\sum_{\mathbf{k}}\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle + g'\sum_{\mathbf{k}}\langle d_{-\mathbf{k}\downarrow}d_{\mathbf{k}\uparrow}\rangle$$

Transforming to the quasi-particle operators, H^{mf}_I can be re-written as

$$H^{mf}_I = \sum_{\mathbf{k}}\Delta_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}\uparrow}\alpha^\dagger_{-\mathbf{k}\downarrow} + \sum_{\mathbf{k}}\Delta'_{\mathbf{k}}\beta^\dagger_{\mathbf{k}\uparrow}\beta^\dagger_{-\mathbf{k}\downarrow} + h.c.) + const. \tag{7}$$

$$\tag{8}$$

Here, $\Delta_{\mathbf{k}} = \frac{\Delta t^2 + \Delta'(\epsilon^+ - \epsilon)^2}{(\epsilon^+ - \epsilon)^2 + t^2}$ and $\Delta'_{\mathbf{k}} = \frac{\Delta' t^2 + \Delta(\epsilon^+ - \epsilon)^2}{(\epsilon^+ - \epsilon)^2 + t^2}$. The two bands are completely decoupled above leading to an identification of Δ and Δ' as the gap functions in the plane and the chain respectively. On the FS $\epsilon\epsilon' = t^2$ and one has a single OP given by $\Delta_{\mathbf{k}} = \Delta'_{\mathbf{k}} = \frac{\Delta'\epsilon + \Delta\epsilon'}{\epsilon + \epsilon'}$. Since ϵ, ϵ' have the same sign on the FS, the only way $\Delta_{\mathbf{k}}$ changes sign (and consequently have a node) along the way on the FS is by having Δ and Δ' out of phase. This is, of course, ensured by the repulsive interaction K between the two bands as discussed above.

Diagonalization of the full Hamiltonian $H_0 + H^{mf}_I$ is achieved using the usual Nambu representation $\psi^\dagger_{\mathbf{k}} = \left(c^\dagger_{\mathbf{k}\uparrow}\, c_{-\mathbf{k}\downarrow}\, d^\dagger_{\mathbf{k}\uparrow}\, d_{-\mathbf{k}\downarrow}\right)$ and writing the mean-field Hamiltonian as $\psi^\dagger_{\mathbf{k}}\mathcal{M}\psi_{\mathbf{k}}$,

where $\mathcal{M}$ is the 4×4 mean-field Hamiltonian matrix. The four eigenvalues are obtained from

$$2E_{\mathbf{k}}^{\pm 2} = \eta + \eta' \pm \sqrt{(\eta - \eta')^2 + 4(\tau^2 + \delta^2)} \tag{9}$$

where, $\eta = \epsilon^2 + \Delta^2 + t^2$, $\eta' = \epsilon'^2 + \Delta'^2 + t^2$, $\tau = t(\epsilon + \epsilon')$ and $\delta = t(\Delta - \Delta')$

On minimization of the mean-field free energy with respect to Δ^* and Δ'^* the gap equations are obtained as (with β as the inverse temperature).

$$\frac{K\Delta + g\Delta'}{gg' - K^2} = \sum_{\mathbf{k}} \left(\frac{\partial E_{\mathbf{k}}^+}{\partial \Delta'} tanh \frac{\beta E_{\mathbf{k}}^+}{2} + \frac{\partial E_{\mathbf{k}}^-}{\partial \Delta'} tanh \frac{\beta E_{\mathbf{k}}^-}{2} \right) \tag{10}$$

and

$$\frac{K\Delta' + g'\Delta}{gg' - K^2} = \sum_{\mathbf{k}} \left(\frac{\partial E_{\mathbf{k}}^+}{\partial \Delta} tanh \frac{\beta E_{\mathbf{k}}^+}{2} + \frac{\partial E_{\mathbf{k}}^-}{\partial \Delta} tanh \frac{\beta E_{\mathbf{k}}^-}{2} \right) \tag{11}$$

These gap equations are solved numerically and the two gap functions, have the usual square root dependence on temperature, but opposite signs. This change of sign of the gap function on the same sheet of the FS has important bearing on the physics of the model.

Since the FS is a combination of contributions from the chain and plane bands, as we move along any one of sheets of the FS the OP changes from Δ to Δ' or vice versa, and hence changes sign. The appearence of OP with different signs can be seen by expanding the Free energy, obtained from MF Hamiltonian (Eqn. 6), about (Δ, Δ') =(0,0) close to the transition.The expression to second order in Δ and Δ' is,

$$F = a|\Delta|^2 + b|\Delta'|^2 + 4c(\Delta\Delta^* + \Delta^*\Delta) \tag{12}$$

with $a = \frac{g'}{gg'-K^2} - u - v - w, b = \frac{g}{gg'-K^2} - u - v + w$,and$c = \frac{K}{gg'-K^2} + v$
where,

$$u = \frac{1}{4} \sum_{\mathbf{k}} \left[\frac{tanh\beta E^+(0,0)}{E^+(0,0)} + \frac{tanh\beta E^-(0,0)}{E^-(0,0)} \right]$$

$$v = \frac{1}{2} \sum_{\mathbf{k}} \frac{t^2}{\sqrt{(\epsilon^2 - \epsilon'^2)^2 + 4t^2(\epsilon + \epsilon')^2}} \left[\frac{tanh\beta E^+(0,0)}{E^+(0,0)} - \frac{tanh\beta E^-(0,0)}{E^-(0,0)} \right]$$

$$w = \frac{1}{4} \sum_{\mathbf{k}} \frac{\epsilon^2 - \epsilon'^2}{\sqrt{(\epsilon^2 - \epsilon'^2)^2 + 4t^2(\epsilon + \epsilon')^2}} \left[\frac{tanh\beta E^+(0,0)}{E^+(0,0)} - \frac{tanh\beta E^-(0,0)}{E^-(0,0)} \right]$$

A nonzero c ensures that there is a single T_c, because whenever one of the order parameters approaches zero, it forces the other to vanish simultanously. Since v can be seen to be positive and the interaction strength K is not large enough ($K^2 < gg'$), the sign of the coefficient of the third term in the expanded free energy above is always nonzero (unless $t = K = 0$) and positive. The free energy is then minimized with the order parameters Δ and Δ' having opposite signs. This, of course, ensures that there is a node on the FS and that there is a single transition temperature. Experimentally, one does indeed see only one specific heat anomaly[2].

Having obtained Δ and Δ' thus, it is natural to look for the sign of the OP on the FS. We show in Fig. 3 how $\Delta_{\mathbf{k}}$ behaves as one moves along the (non-interacting) FS. The consequent node positions on the FS are shown in Fig. 1 for optimal values of g, g' and K (that fit the T_c, see discussion below). The nodes are very close to the (π, π) direction as seen experimentally for $YBa_2Cu_3O_7$, a feature shared by the d-wave OP. We also calculate the position of the nodes as a function of doping (inset of Fig. 1). The node positions turn out to be not very sensitive to doping x in $YBa_2Cu_3O_{6+x}$, varying within $\pm 10^o$ about 45^o i.e., (π, π) direction. Although there is no experimental data to compare it with presently, this remains a testable prediction of the model at hand.

It is in the fitness of things that at this point we calculate the dependence of the superconducting transition temperature T_c as a function doping x shown in Fig. 4. We have used as fitting parameters g, g' and K, while the band parameters have already been fixed to fit the ARPES data as discussed earlier. We chose the values of these parameters such that g, g' and K are within reasonable limits giving T_c at $x = 1$ around 100^oK. The slightly higher value (100^oK as compared to the experimental value $\simeq 90^o$) that we have chosen is to account for the strong fluctuations that are present in these systems owing to their intrinsic low dimensionality[19]. A reduction of T_c by about 10 to 20 percent due to fluctuations is generally observed. The optimal values, thus fixed, turned out to be 225, 140 and 125 meV, with $t = 50meV$ fixed earlier. The T_c is maximum at $x = 1$ where the Fermi level is closest to the van Hove singularity (Fig. 2). As one moves away from this filling, the DOS at the Fermi level drops drastically and then moves over a plateau. The T_c versus x curve follows this pattern as expected. We have also studied the behaviour of T_c as a function of the interaction parameters g, g' and K and the interband hopping strength t. The variations of T_c with g and g' show the usual BCS behaviour. Interesting variations are observed in the dependence of T_c on K and t. As the two gap parameters Δ and Δ' have opposite signs, and t induces band mixing, T_c goes down quite dramatically with t. Conversely, K works

counter to this and so pushes the T_c up showing up as a minimum (that moves towards lower temperature as t is brought down from 50 to $15meV$) followed by the usual rise as expected in a two band model for superconductivity[18].

The two different order parameters in our model are not related by any symmetry, except that they have different signs. The c-axis Josephson current, therefore, does not cancel out completely as in the case of a d-wave order parameter, although partial cancellation occurs due to the opposite signs of Δ and Δ' resulting in a small (compared to an s-wave OP) but finite current as seen in experiments[8]. We found the node on the FS close to the (π, π) direction, which is not very sensitive to the doping concentration. The appearance of the node on the FS ensures a linear temperature dependence of penetration depth and *low energy excitations* seen in the thermodynamic measurements. The order parameter in $a-$ ($b-$) direction is mainly chain (plane) like and hence provide a natural explanation for the observed phase change π in SQUID experiments.

The s-wave order parameter is weakly influenced by impurities (Anderson theorem). In a $d-$wave superconductor, however, scattering between lobes of different sign on the FS reduces the T_c much faster. This averaging out of the sign and consequent sensitivity towards non-magnetic impurities will occur in the present model as well, albeit at a much slower rate than in the $d-$wave case. Sign of OP changes in the present model only by scattering from planes to chains, involving strong scattering processes only. Sensitivity of T_c towards non-magnetic impurity will, therefore, be intermediate between an $s-$ and a $d-$ wave superconductor in our case[20], as seen in the high T_c materials[2, 11]. The superfluid density, obtained by calculating the leading order fluctuations over the mean-field state gives an anisotropic penetration depth[20].

In the $YBCO$ system, the unit cell contains two planes and one chain. So that a more realistic model would be where these additional features are present. It is important to note, however, that the conclusions of the present model are not very sensitive to whether we work with a chain and a plane, two or more planes or chains, or a combination of them. This a simple model that incorporates the effect of having more than one OP residing on different bands that are coupled and shows that with the correct choice of phase of the different OP can capture many of the unusual features of the symmetry of OP in these systems. It would be nice to see experimental results on the position of the node(s) on the FS as a function of doping. In the $d-$wave case, since the position is dictated by symmetry, there will be no change as the FS changes shape, while in any of the $s-$wave models, it will. Though in our model, for a range of doping, the sensitivity is not too strong.

In conclusion, we have shown that it is possible to understand many of the contradictory experimental evidences from a simple and realistic model applicable to layered superconductors.

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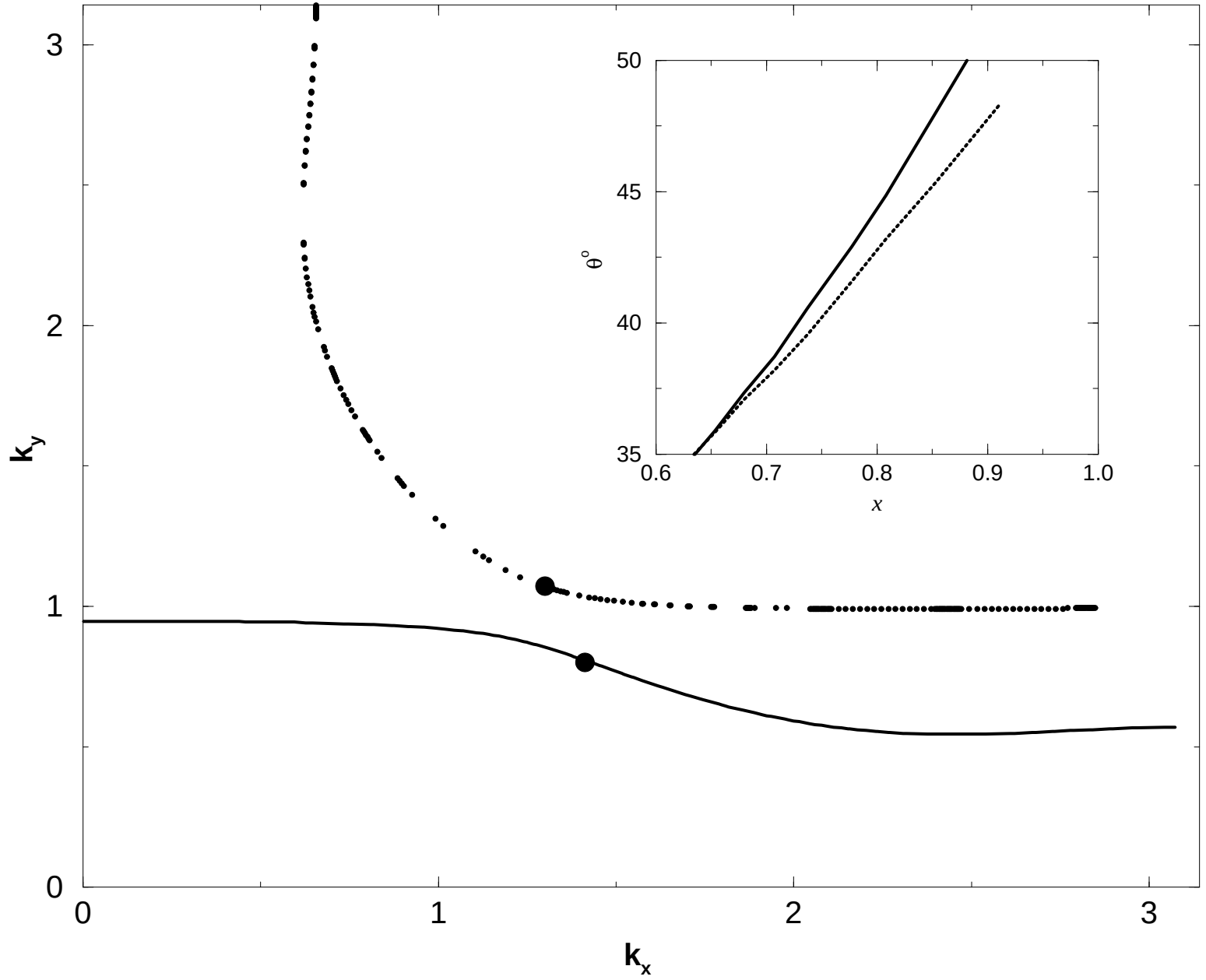
FIGURE CAPTIONS

Fig. 1 The two sheets of FS are shown in the first quadrant of the BZ.The dotted(solid) line corresponds to $\epsilon^- = 0$ ($\epsilon^+ = 0$). The filled circles show the position of nodes of OP on FSat $x = 0.9$. The variation of the node positions on FS with x is shown in the inset.

Fig. 2 The DOS for noninteracting quasiparticles is shown. vHS is around 10 meV below the Fermi Energy. The inset shows the partialal DOS, where the dotted(solid) line corresponds to the ϵ^- (ϵ^+) band.

Fig. 3 The anisotropic OP comes out to be same in two different sheets of FS.In the figure the dashed (solid) line shows how $\Delta_k (= \Delta_k{}')$ behaves on FS corresponds to $\epsilon^- = 0 (\epsilon^+ = 0$) at $x = 0.9$. Clearly two point nodes are visible.

Fig. 4 The behaviour of T_c with doping concentration, shown in this figure is somewhat similar to the experimental curve.The platue around $x = 0.8$ is prominant and the max. T_c about $x \approx 1$ is because of the presence of vHS there.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θ^o
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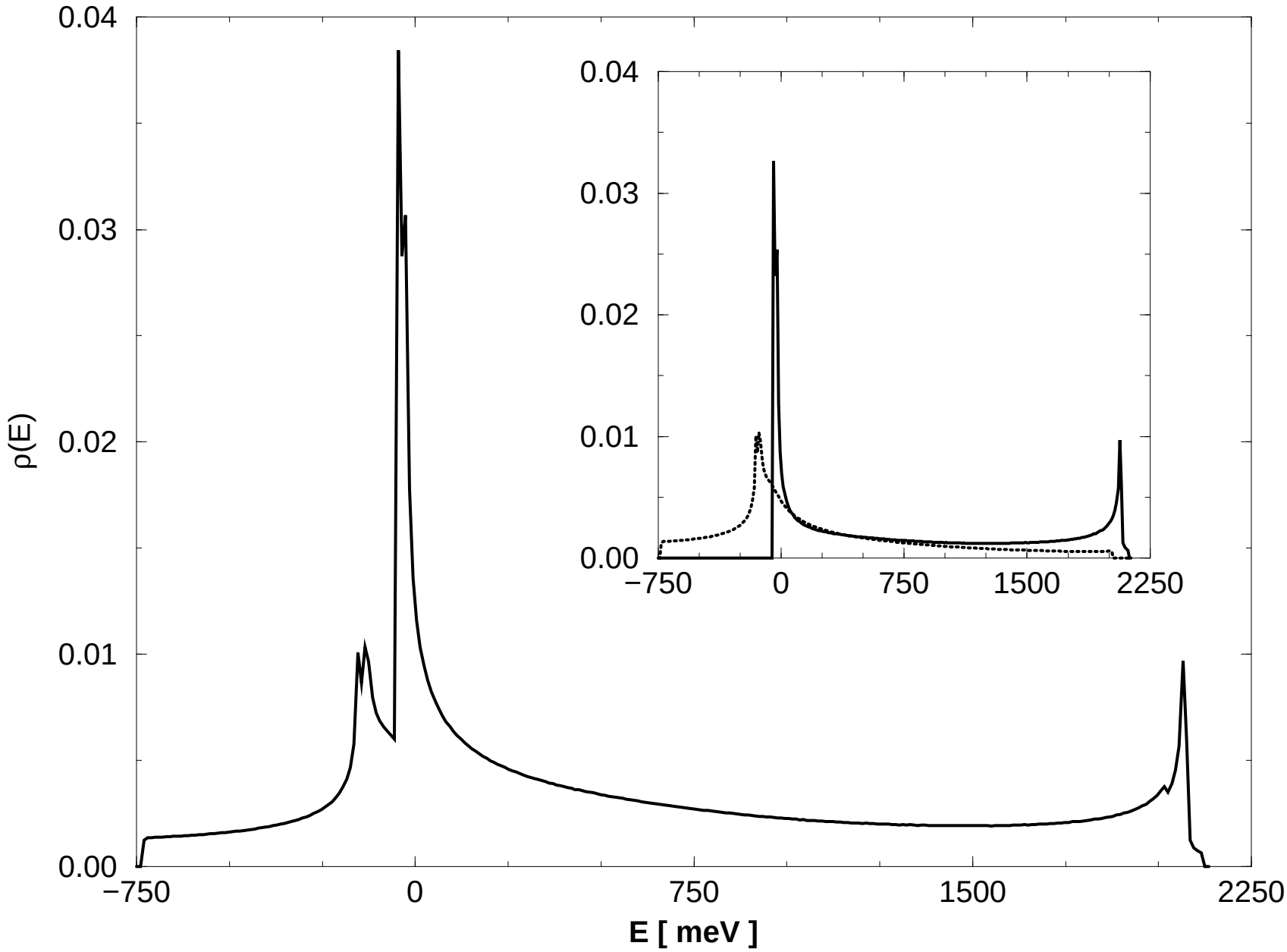
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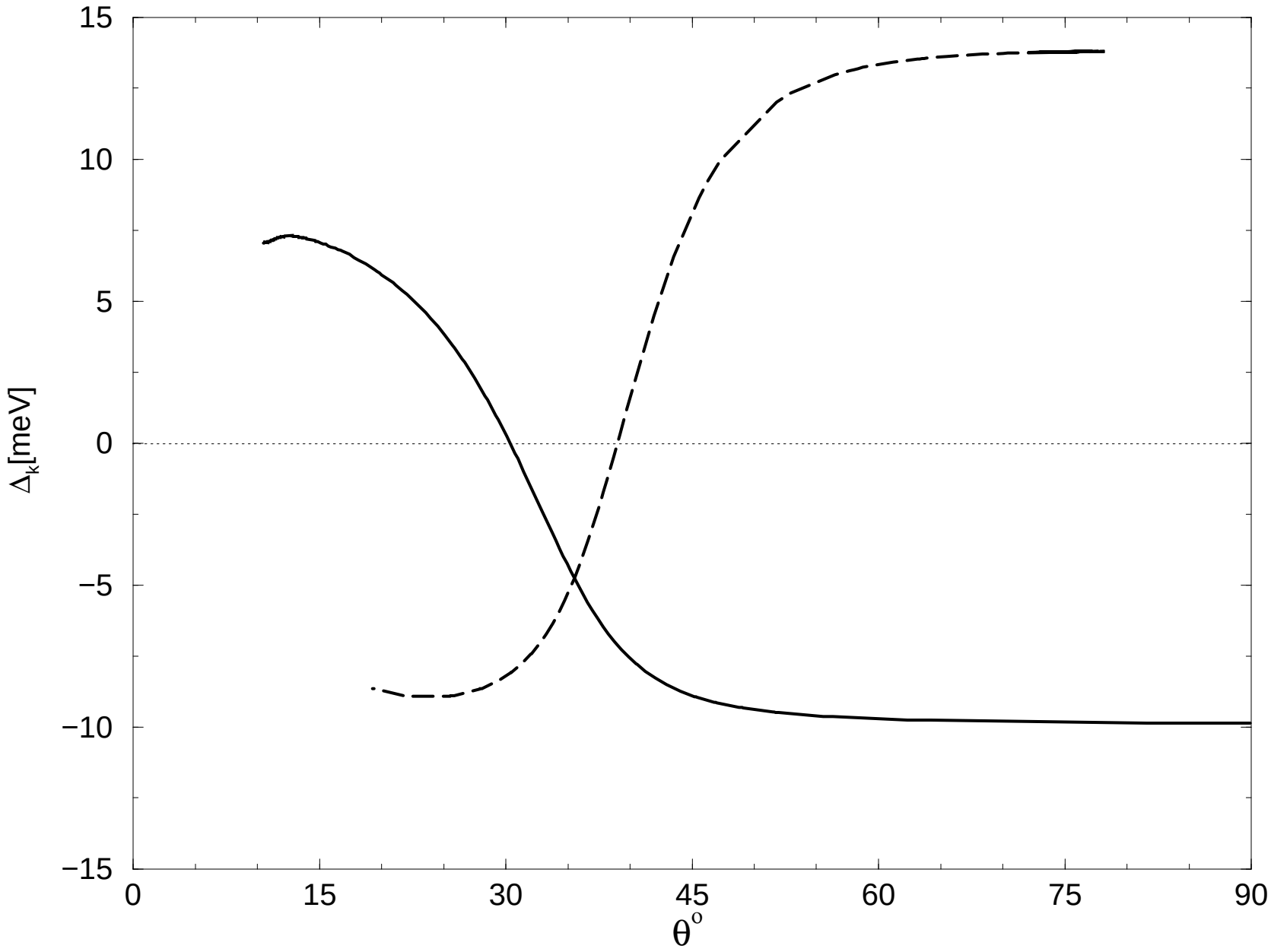
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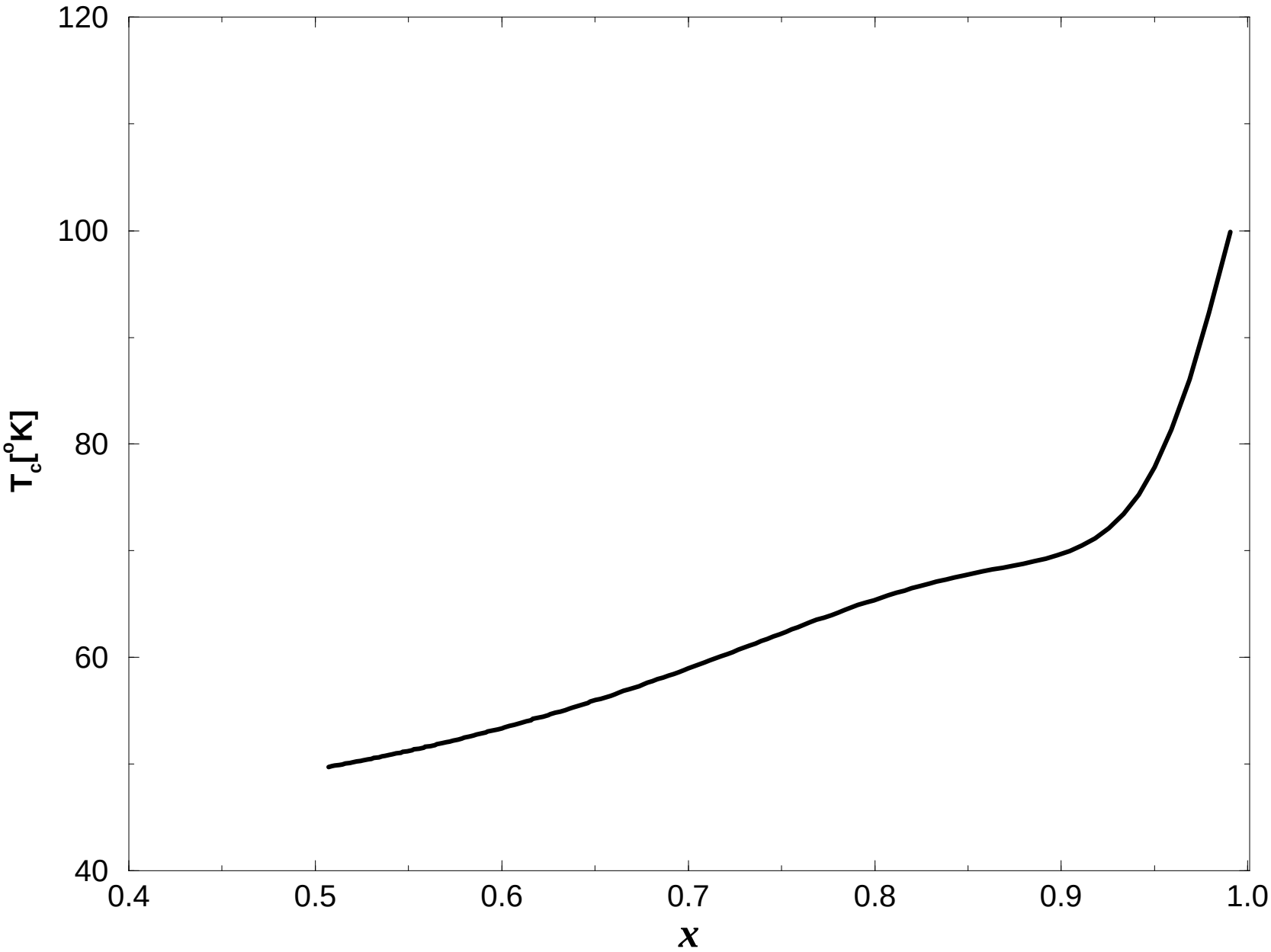
θ°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100
80
60
40
T_c[°K]
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x